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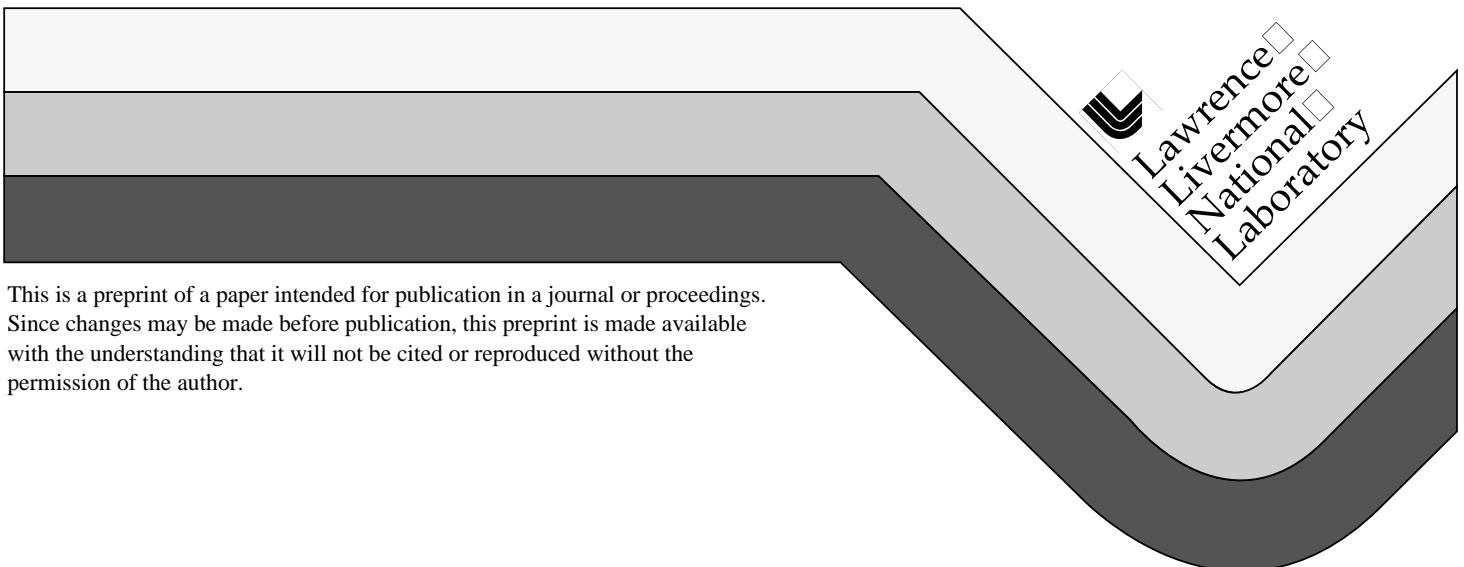
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# **Remediation Tradeoffs Addressed with Simulated Annealing Optimization**

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## **Abstract**

Escalation of groundwater remediation costs has encouraged both advances in optimization techniques to balance remediation objectives and economics and development of innovative technologies to expedite source region clean-ups. We present an optimization application building on a pump-and-treat model, yet assuming *a priori* removal of different portions of the source area to address the evolving management issue of more aggressive source remediation. Separate economic estimates of *in-situ* thermal remediation are combined with the economic estimates of the subsequent optimal pump-and-treat remediation to observe tradeoff relationships of cost vs. highest remaining contamination levels (hot spot). The simulated annealing algorithm calls the flow and transport model to evaluate the success of a proposed remediation scenario at a U.S.A. Superfund site contaminated with volatile organic compounds (VOCs).

## **1 Introduction**

Many researchers integrate optimization and groundwater transport modeling to search for efficient remediation (e.g. [1]). Previous nonlinear, large-scale, optimal, remediation design at Lawrence Livermore National Laboratory (LLNL) has been based on 2-D groundwater flow and transport models (GFTM) and artificial neural networks (ANNs) trained to predict GFTM outcomes (Dowla and Rogers[2], Rogers and Dowla[3], Rogers et al.[4], Johnson et al.[5]). The search has been directed by a genetic algorithm (GA) or simulated annealing (SA) optimization. This approach has advantages of 1)  $10^6$  increase in pumping pattern assessment speed during the searches and

sensitivity analyses for the 2-D LLNL work, 2) freedom from sequential runs of the GFTM (enables workstation farming), and 3) recycling of the knowledge base (i.e. GFTM runs to train the ANNs (see Website:<http://www-ep.es.llnl.gov/www-ep/esd/ssstrans/pmp.html>). With our recent access to a Dec Alpha cluster (single GFTM runs reduced from about 2 hr to 10 min), we opted to use an SA algorithm which called the full GFTM for a pumping pattern assessment.

Expense and long duration of pump-and-treat remediation has encouraged innovative *in-situ* technologies. LLNL has explored thermal and biofilter technologies (see Website:<http://www-ep.es.llnl.gov/www-ep/aet/ACI/aci-home.html>). Hydrous Pyrolysis (HP) destroys contamination *in situ* by thermal oxidation from steam injection. Biofilters complement steam injection by forming a permeable wall destroying contaminants as they are pushed through it.

A 3-D nonisothermal code has been used in HP process simulations to gauge field deployment feasibility at LLNL site (e.g. Knapp[6]). We wanted to address how resources might be balanced between pump-and-treat remediation and more aggressive *in-situ* source remediation. We do not now have a field-scale nonisothermal model to link to the optimization. As an approximation we consider three cases of increasing initial source remediation with their associated economic estimates to implement HP.

Tradeoff is used here to indicate how emphasis of one objective compromises performance in another conflicting objective. For our three cases we have constructed tradeoff curves based on the SA searches to compare the economic feasibility of *in-situ* removal of the contaminated source area vs. pump-and-treat remediation of the entire plume.

## 2 Western USA Superfund Example

We consider a hypothetical example drawn from field measurements of VOC groundwater contamination at a well-characterized Superfund site at LLNL. Earlier work (e.g. Johnson et al.[5]) optimized a well pump-and-treat/ injection strategy using a 2-D numerical GFTM. A 28-well basecase remediation obtained by expert trial-and-error modeling was optimized. Several pumping patterns were found in the GA-ANN search which contained the plume at estimated savings of \$102-\$114.2 over 50 yr of remediation and extracted as much or more contaminant mass than the basecase.

In this work the same 2-D hybrid finite-element/finite GFTM, SUTRA (e.g. Voss,[7]), was used to evaluate the outcome of

remediation scenarios. The upper 200 ft of the saturated zone was modeled in a vertically averaged, steady-state, saturated approach. A 2,385 element grid was superimposed on the square mile site of LLNL and approximately 15 surrounding square miles. Elements ranged from 76 m on a side in the center to 610 m on a side on remote northwest boundaries. The model was calibrated to a larger regional model extensively calibrated to water-table conditions, known source and sink phenomena, and other field observations (e.g. Thompson et al., [8]). General direction of groundwater flow is to the west. Flow boundaries were no-flow fault zones to the northeast and southeast, with flux boundaries east and distantly downgradient to the west.

Consider 3 cases: Case A: pump-and-treat from initial condition to final, no accelerated source cleanup (Fig. 1), Case B: an instantaneous source removal of concentration > 500 ppb then pump-and-treat of remaining concentration (Fig. 2), and Case C: an instantaneous source removal of concentration > 350 ppb then pump-and-treat of remaining concentration (Fig. 3). The instantaneous removal is an idealization to represent the fast action of HP relative to pump-and-treat. *In-situ* HP was estimated from LLNL field experience to cost \$35 per cubic yard. We refer to the cost of initial source cleanup with HP as the Pluck Cost (i.e. cost of plucking a small area, or cookie, out of the contaminated area. Pluck Cost for the cases is estimated as \$0, \$11 m, and \$26 m, respectively.

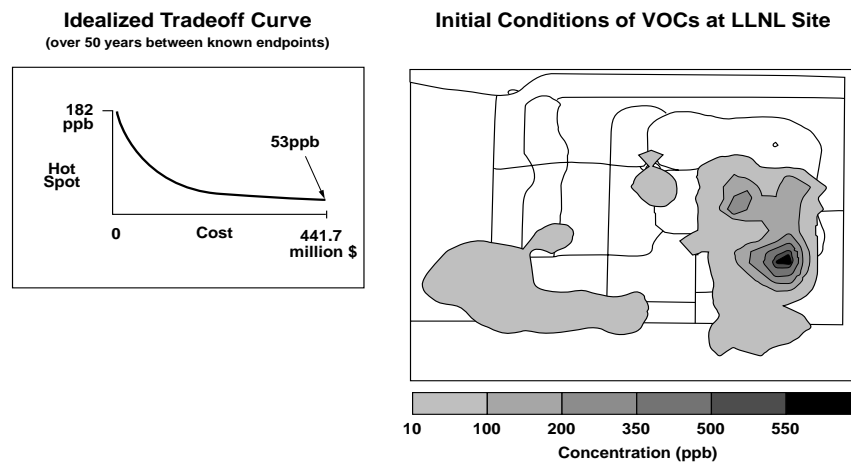


Figure 1: Case A: No Cookie (Pluck Cost \$0). Hot spot is greatest remaining concentration, cost and hot spot are after 50 yr of remediation.

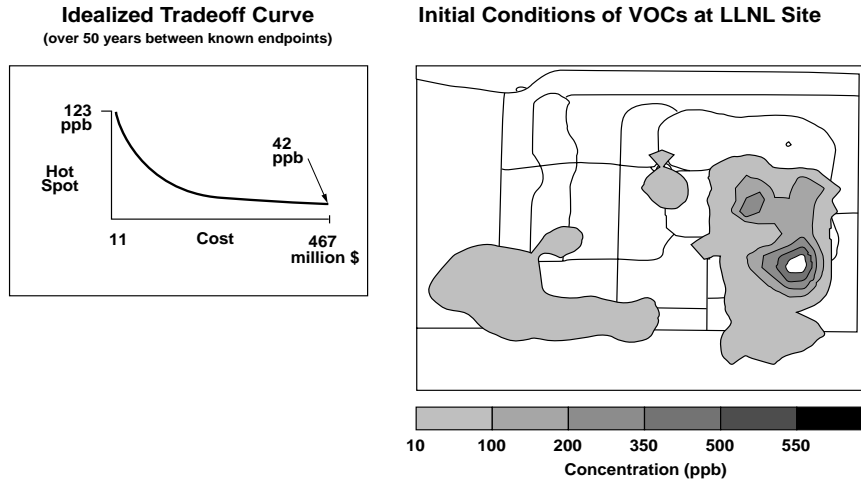


Figure 2: Case B: Cookie Cut Out of > 500ppb  
(Pluck Cost \$11 million).

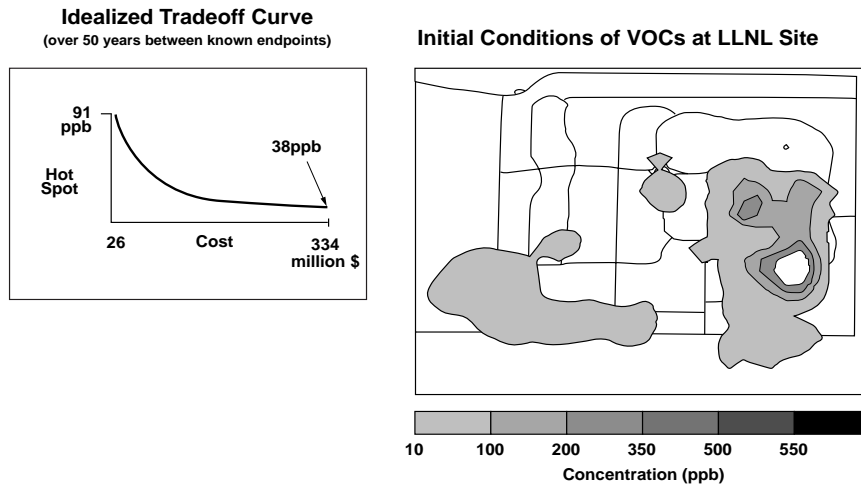


Figure 3: Case C: Cookie Cut Out of > 350ppb  
(Pluck cost \$26 million).

The idealized tradeoff curves connect known endpoints of 1) highest contamination or hot spot after 50 yr if nothing is done after Pluck Cost and 2) search results for an optimal pump-and-treat strategy of lowest hot spot after 50 yr of unlimited spending. An SA search will start with possible well patterns randomly scattered between the endpoints. At the end of the search the patterns will cluster towards the tradeoff curve which represents the best solutions.

## 3 The Approach

### 3.1 Optimization driver

We employed the SA algorithm (e.g. Metropolis[9], Kirkpatrick[10], Reeves[11]). SA evolved in analogy to the annealing of solids where initial energy of a system is raised to allow molecules to be mobile; later the system is cooled to a lower energy crystalline form. A search objective such as cost is mapped onto the energy of the system and the feasible solutions onto the state of the system. At early times perturbations to feasible solutions may be large; as temperature decreases change is curtailed. Probabilistic rules control the number of changes at given temperature steps. This method has found success in large-scale optimization applications including groundwater ones (e.g. Dougherty and Marryott[12], Rizzo and Dougherty[13]).

We use two main probabilistic rules, probability of change in creating a new possible pumping pattern and probability of acceptance of a new pattern if it is not better than the last pattern. Decision variables are whether 30 preselected pumping wells are off or on at their full capacity. Note any mention of temperature here refers to the SA search framework; it has no relation to the thermal remediation. The probability of change, or how many of the 30 components were changed in creating a new pattern was set to  $30 * \text{the temperature}$ , with the decrement of temperatures, or cooling schedule, set to the often used relationship of  $\text{new temperature} = \text{old temperature} * 0.9$ . Probability of acceptance was an exponential function of the current temperature and difference between old pattern success and new pattern success (step 4 below).

About 40 SA searches were run to examine search behavior and appropriate temperature area of interest. A possible temperature scale of 1-0 was narrowed to .25 - .01. The runs revealed the need for a magnification factor (step 3 below) as the small differences between the success of our patterns led to search stagnation. We designed our SA algorithm to benchmark against a GA; thus, our formulation has an opposite sign to the traditional decrease of the energy of the system. Our objective function increases like the fitness of the GA formulation. New pattern selection may be simplified in the following steps: 1) generation of a new pumping pattern, 2) if success of new pattern > success of old pattern then keep new pattern else, 3) worsening factor = (success of old pattern - success of new pattern) \* magnification factor, 4) probability of acceptance =  $\exp(-\text{worsening factor})$

factor/current temperature); 5) generate a random number, 6) if random probability < acceptance probability, keep new pattern.

### **3.2 Objective Function Formulation and Search**

The optimization objectives were to minimize remediation cost and minimize the hot spot after 50 yr of pump-and-treat remediation. There are innumerable combinations of remediation objectives; we have chosen one of interest to us. Injection was not a decision variable, 75% of the extracted water was reinjected to the east, hydraulically upgradient from the extraction wells. Earlier work found mid-site injection resulted in large pumping/treatment costs of only lightly contaminated water. Total injection was capped at 50 gpm.

The cost function summed well construction/maintenance and surface treatment costs assuming constant pumping over 50 yr. Capacity varied from well to well. An injection well was estimated to cost \$433,000 including well construction, testing, piping, operational and maintenance costs. Treatment costs were estimated at \$.00725 per liter and operational/maintenance costs at \$.00006 per liter.

It is an art to unravel how weights of individual components of the objective function affect the final recommended solutions. We used constant weights of objective function components with hot spot weighted double the cost. The objective function thus was formulated as  $(1 - \text{normalized value of the cost of remediation over 50 yr}) + 2 * (1 - \text{normalized highest remaining hot spot})$ . Each SA search used 800 to 1000 GFTM calls. At each temperature level 100 new patterns were evaluated. Any time a pumping pattern with a fitness score above 2.45 appeared in the search, it was saved for later analysis.

### **3.3 Construction and discussion of tradeoff curves**

Our formulation involved a given number of wells at set capacities, so our total costs fell into distinct categories. In construction of Tradeoff Curve A solutions resulting in the lowest hot spot after 50 yr for each cost category were added to their associated Pluck Costs (Fig. 4). Each of the curves has a similar slope in the area where our SA search focused, roughly 1 ppb decrease in hot spot remaining per \$10 m investment. The real gain appears to come in the initial expenditure. Note initial expenditure of approximately \$ 11 m in Case A, results in a 30 ppb reduction after 50 yr. To use the same \$11 m for *in-situ* source remediation (Case B) can result in bringing the hot spot down 60 ppb. Comparing an initial pump-and-treat



expenditure on Case A we see approximately a 60 ppb lowering of the hot spot, whereas devoting the first \$25 m to *in-situ* remediation (Case A) would lower the hot spot approximately 90 ppb. Note the lowest hot spot level in this area of the curve is approximately 63, 47, and 39 for Case A, Case B, and Case C, respectively.

Another way to examine this data is shown in Tradeoff Curve B which was constructed by estimating the difference in the total cost of remediation between the different cases for a selected hot spot on Tradeoff Curve A. More resolution would have been useful along the Tradeoff Curve A to improve the accuracy of Tradeoff Curve B; however, some useful generalizations may be obtained from this exercise. If one is interested in getting the hot spot below 60, aggressive hot spot remediation (Case C) is probably the best choice. Between about 60 and 90 ppb, Case B and Case C are roughly equivalent, above that Case B is probably the better choice. This analysis suggests for this combination of remediation objective, proactive source remediation is overall more cost effective, especially relative to pump-and-treat by itself.

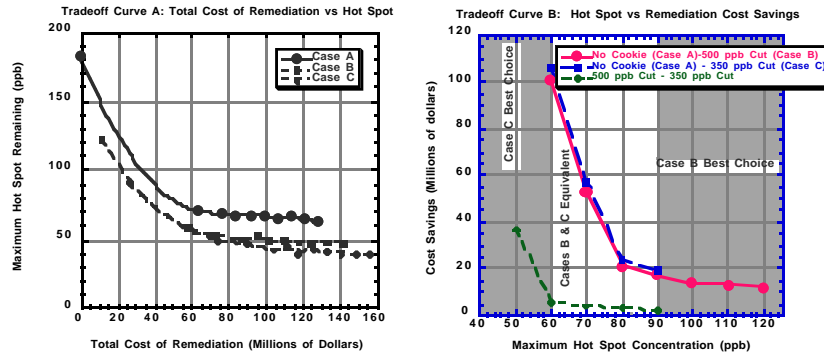


Figure 4: Tradeoff Curves

## 4 Conclusions

High remediation costs and new alternatives encourages broader optimization formulation, increased complexity of transport to include *in-situ* technology dynamics, and more efficient optimization methodologies. We have used here the robust SA algorithm for field-scale multiple objective searches and used the results to construct tradeoff curves to aid setting management priorities.

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